

Systematics of the Quadrupole-Quadrupole Interaction and Convergence Properties

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Our main concern in this work is to show how higher shell admixtures affect the spectrum of a $Q \cdot Q$ interaction. We first review how, in the valence space, the familiar SU(3) result for the energy spectrum can be obtained using a coordinate space $Q \cdot Q$ interaction rather than the Elliott one which is symmetric in \mathbf{r} and \mathbf{p} . We then reemphasize that the Elliott spectrum goes as $L(L+1)$ where L is the orbital angular momentum. While in many cases this is compatible with the rotational formula which involves $I(I+1)$, where I is the total angular momentum, there are cases, e.g. odd-odd nuclei, where there is disagreement. Finally, we consider higher shell admixtures and devise a scheme so as to obtain results, with the $Q \cdot Q$ interaction, which converge as the model spaces are increased. We consider not only ground state rotational bands but also those that involve intruder states.

I. INTRODUCTION

There have been studies in the past of the quadrupole-quadrupole ($Q \cdot Q$) interaction in multishell spaces using the non-compact symplectic groups [1,2]. Most of the focus of these studies has been on the ground state rotational bands, the γ vibration bands ($K=2$), the giant quadrupole resonances and the effective charges. In this work we wish to discuss the problems of extending the above studies to other topics such as intruder states, odd-odd nuclei, etc. We feel that there has not been any clear discussion of how higher shell admixtures affect the overall low lying spectrum in a given nucleus, nor of how the low lying bands of odd-odd nuclei are described with this interaction. Also we have recently shown how to restore Elliott's SU(3) results [3] with a coordinate space quadrupole-quadrupole interaction rather than one that is symmetric in position and momentum. We will show that this is of more than academic interest. We also discuss differences between Elliott's SU(3) approach [3–6] and the rotational model. The problem of convergence with a $Q \cdot Q$ interaction is discussed in the last section.

The $Q \cdot Q$ interaction has a long history, the early part of which can be found by reading excerpts from the text book by A.M. Lane [7], and for recent applications the book by I. Talmi is recommended [8].

Following the notation of Golin and Zamick [9] we define the multipole-multipole interaction (including isospin) as

$$V(r) = -\chi [(2L+1)(2T+1)]^{1/2} [Y^L(1)Y^L(2)]^0 f(r_1)f(r_2) [\delta_{T,1}[\tau(1)\tau(2)]^0 + \delta_{T,0}] \quad (1)$$

where $-\sqrt{3}[\tau(1)\tau(2)]^0 = \tau(1) \cdot \tau(2)$.

The detailed expressions for the unnormalized antisymmetrized matrix elements of this interaction are given in the above mentioned work of Golin and Zamick [9]. The expression is fairly complicated, involving Racah coefficients. However the expression for the direct part of the particle-hole matrix element (ph) for a ph state with total angular momentum I and isospin T' is much simpler. The expression is proportional to $\delta_{I,L}\delta_{T,T'}$ and indeed there is no other I, T' dependence. Thus, if one ignores the exchange part of the interaction one has a simple schematic interaction. Thus, as Lane describes [7], we can use this interaction to describe collective vibrational spectra.

The pairing plus quadrupole model was very popular and has been used by Kisslinger and Sorensen [10], Baranger [11] and Ikeda et al. [12] around 1960, especially to describe the first excited 2^+ state in vibrational nuclei. It can also be applied to giant quadrupole resonances as emphasized by Bohr and Mottelson [13]. Here, the schematic model of Brown and Bolsterli [14] can be used. One can also couple a particle to the giant quadrupole resonance and get an $E2$ effective charge. If one uses the selfconsistent strength for χ as given by Bohr and Mottelson one finds that the isoscalar polarization charge $\delta e_p + \delta e_n$ is equal to the bare charge in an RPA calculation.

In a different direction Elliott has shown [3] that a suitably defined $Q \cdot Q$ interaction leads to rotational spectra in an open shell nucleus with single-particle states defined by an isotropic three-dimensional harmonic oscillator potential. His interaction is

$$V_E = -\frac{\chi}{2} \sum_{ij} \left(\frac{Q^r + Q^p}{2} \right) \cdot \left(\frac{Q^r + Q^p}{2} \right) \quad (2)$$

Note that it includes $i = j$ terms and that his quadrupole operator is symmetric in position and momentum and this ensures that there will be no mixing of major shells. This will be discussed in more detail later. Elliott noted that the Casimir operator for the SU(3) group is

$$\tilde{C}_2 = Q \cdot Q - 3L \cdot L \quad (3)$$

From this he obtained the famous expression for the energy levels for a rotational band for states with SU(3) quantum numbers λ, μ

$$\langle V_E \rangle = \bar{\chi} [-4 (\lambda^2 + \mu^2 + \lambda\mu + 3(\lambda + \mu)) + 3L(L + 1)] \quad (4)$$

For fixed λ, μ one gets the spectrum of a rotational band, but going as $L(L + 1)$ rather than $I(I + 1)$.

We thus see that the $Q \cdot Q$ interaction has been used to make more transparent how nuclear collectivity arises despite the fact that the shell model with its implications of single particle motion seems to work. It should be added that one can regard $Q \cdot Q$ as the long range part of a more realistic interaction. This has been shown by many authors and we recommend Talmi's book [8] for a nice detailed derivation of this.

II. MOMENTUM DEPENDENT Q.Q INTERACTIONS AND THE STABILITY PARADOX

It is of general interest to know how momentum dependent interactions affect nuclear deformations. For example the Skyrme interaction contains the momentum dependent terms $k'^2 \delta(\mathbf{r}_1 - \mathbf{r}_2) + \delta(\mathbf{r}_1 - \mathbf{r}_2) k^2$ and $\mathbf{k}' \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k}$ [15–17]. The presence of those terms leads to an effective mass $m^* < m$ in the nucleus. The rationale given to those momentum dependent terms is that they simulate the finite range nature of the nucleon-nucleon interaction. However, since the Skyrme interactions are phenomenological they may be simulating more fundamental momentum dependence of the nucleon-nucleon interaction.

The effect of the momentum dependent terms is known for the energy of the isoscalar giant quadrupole resonance [18,13]

$$E^* = \sqrt{2} \hbar \omega \sqrt{\frac{m}{m^*}} . \quad (5)$$

The effect on the ground state deformations is not so well known.

Another example of momentum dependence is the Hamiltonian used by Elliott to obtain SU(3) results [3]. This Hamiltonian is symmetric in position and momentum coordinates

$$H = \sum_i \left(\frac{p^2}{2m} + \frac{1}{2} m \omega^2 r^2 \right) - \frac{\chi}{2} \sum_{ij} \left[\frac{Q^r + Q^p}{2} \right] \cdot \left[\frac{Q^r + Q^p}{2} \right] , \quad (6)$$

$$Q_\mu^r = r^2 Y_{2,\mu}(\Omega_r); \quad Q_\mu^p = b^4 p^2 Y_{2,\mu}(\Omega_p); \quad (b^2 = \hbar/m\omega) . \quad (7)$$

We also define for convenience

$$Q^E = \frac{1}{2} (Q^r + Q^p) . \quad (8)$$

The momentum terms prevent $\Delta N = 2$ mixing between major shells. Although the original intention for this Hamiltonian is for valence nucleons in a given major shell, let us use it here as an extreme example of a momentum dependent Hamiltonian which is symmetric in \mathbf{r} and \mathbf{p} and perform a Hartree-Fock calculation with it.

In general, for any interaction in a deformed Hartree-Fock calculation the condition for stability can be formulated as follows [19]

$$\left\langle \sum_i (Q_p) \right\rangle = 0 , \quad (9)$$

where Q_p is the quadrupole moment operator in momentum space

$$Q_p = b^4 \sqrt{\frac{5}{16\pi}} (2p_z^2 - p_x^2 - p_y^2) . \quad (10)$$

However, since the Hamiltonian is symmetric in \mathbf{r} and \mathbf{p} , so is the Wigner distribution function [20]. This leads to the conclusion $\langle \sum_i Q_r \rangle = 0$, i.e., the expectation value of the usual quadrupole moment also vanishes. But then this goes against the common belief that the Elliott model supports rotational motion.

A way out of this dilemma is to do, as we have done, go back to the \mathbf{r} space interaction $Q^r \cdot Q^r$ and note that we can still get the SU(3) results by including in the single-particle energies, not only the contribution from the $i = j$ term in the sum

$$\frac{1}{2} \sum_{i,j} Q^r(i) \cdot Q^r(j)$$

but also the particle-core interaction [21,22]. In these references it was noted that $Q^r \cdot Q^r$ and $Q^E \cdot Q^E$ do not give the same results in a valence space even if one uses harmonic oscillator wave functions unless the particle-core interaction is included. We can write

$$\frac{1}{2} \sum_{ij} Q(i) \cdot Q(j) = \sum_{i < j} Q(i) \cdot Q(j) + \frac{1}{2} \sum_i Q(i) \cdot Q(i) . \quad (11)$$

For the first term one does get the same result for $Q = Q^E$ and $Q = Q^r$ in a given N shell. However this is not the case for the second $i = j$ term. Using $Q = Q^r$ one only gets 2/3 of the value obtained with $Q = Q^E$. We have however shown [21,22] that the remaining 1/3 comes from the (exchange) interaction of the valence nucleon with the core.

Just to clarify things, the diagonal part of $Q^r \cdot Q^r$ and the particle-core interaction are the terms that give the single particle splittings $\Delta_{N(\ell,\ell')}$ for different ℓ values in a major shell. In order to get the SU(3) results of Elliott one must have such a single particle splitting as well as the two-body $Q \cdot Q$ interaction between the valence nucleons. The main difference then between $Q^E \cdot Q^E$ and $Q^r \cdot Q^r$ is that with the former all the single particle splitting comes from the $i = j$ part of $Q^E \cdot Q^E$, whereas with $Q^r \cdot Q^r$ two thirds comes from the $i = j$ part and one third from the particle-core interaction. In more detail the expressions for the single particle splitting between $N\ell$ and $N\ell'$ states are [22]

$$\Delta_{N(\ell,\ell')}^1 = 2\bar{\chi} [\ell(\ell+1) - \ell'(\ell'+1)] ,$$

$$\Delta_{N(\ell,\ell')}^2 = \bar{\chi} [\ell(\ell+1) - \ell'(\ell'+1)] ,$$

where the $\Delta_{N(\ell,\ell')}^1$ comes from the $i = j$ part of $Q^r \cdot Q^r$ and $\Delta_{N(\ell,\ell')}^2$ comes from the particle-core interaction.

III. I(I+1) VS L(L+1) FOR ROTATIONAL BANDS

In this Section we stay in the valence space and make a comparison of Elliott's SU(3) results [3–6] with results of the rotational model [13]. We feel that it has not been sufficiently emphasized that one finds cases where these two models yield different results for the behavior of rotational bands.

In the rotational model the formula for the energy of a state in a rotational band with total angular momentum I is given by [13]

$$E_I = E_0 + \frac{\hbar^2}{2I} \left[I(I+1) + \delta_{K,1/2} (-1)^{I+1/2} (I+1/2) a \right] \quad (12)$$

where a is the decoupling parameter given by $a = - \left\langle K = 1/2 | J_+ | \overline{K = 1/2} \right\rangle$ and where if $|K\rangle = \sum_j C_{j,K} \phi_{j,K}$ then $|\bar{K}\rangle = \sum_j C_{j,K} (-1)^{j+K} \phi_{j,-K}$.

As noted by J.P. Davidson [23] for an odd-odd nucleus with $K_n = \pm 1/2$, $K_p = \mp 1/2$, ($K = 0$), there is an additional term $(-1)^{I+1} a_p a_n \delta_{K,0} (\delta_{K_p,1/2} \delta_{K_n,-1/2} + \delta_{K_p,-1/2} \delta_{K_n,1/2})$ (See also a recent review by Jain et al. [24]). For even-even nuclei, and for odd-even and even-odd nuclei with $K \neq 1/2$, one gets the familiar $I(I+1)$ spectrum [13].

It is generally thought that the Elliott SU(3) model also gives an $I(I+1)$ spectrum. A careful reading of the papers however shows that one really gets an $L(L+1)$ spectrum, where L is the orbital angular momentum [3–6]. In this work we wish to point out that to fully convey the similarities and differences of the Elliott model and the

rotational model, one should consider not only even-even nuclei, but also even-odd (odd-even) and especially odd-odd nuclei. The latter are usually not considered in the standard textbooks.

The point we make in this section is that the spectrum in the SU(3) model is indeed $L(L+1)$ in all of the above instances. This leads to several cases:

(a) **Rotational bands where the spin S is equal to zero.** In this case $I = L$ and one gets an $I(I+1)$ spectrum.

(b) **$K = 1/2$ bands of even-odd (odd-even) nuclei.** Here again the SU(3) spectrum is of $L(L+1)$ type. The Elliott formula is the same as the rotational formula [1] including the decoupling term evaluated in the asymptotic limit. Again, we have consistency between the two approaches.

(c) **Odd-odd nuclei.** Here again the SU(3) spectrum is $L(L+1)$. There are some cases here where one gets a behavior which is not consistent with the rotational formula.

We have performed shell model calculations with all possible configurations in a given major shell using the interaction $\sum_{i<j} Q(i) \cdot Q(j)$ where, in order to get Elliott's SU(3) results we must, as mentioned in Section II, also add single-particle splittings. Therefore, in the $1s-0d$ shell we have $\epsilon_{0d} - \epsilon_{1s} = 18\bar{\chi}$ and in the $1p-0f$ shell we have $\epsilon_{0f} - \epsilon_{1p} = 30\bar{\chi}$, where $\bar{\chi} = (5b^4/32\pi)\chi$ with b the oscillator length parameter $b^2 = \hbar/m\omega$ [21,22].

The same results can of course be obtained from the Elliott SU(3) formula for the energies given in Eq.(4)

One has the further rules [3–6]:

Let $\bar{\lambda}$ be the maximum of λ and μ , and $\bar{\mu}$ the minimum. Then $K_L = \bar{\mu}, \bar{\mu} - 2, \dots, 1$ or 0 and

- $L = K_L, K_L + 1, \dots, K_L + \bar{\lambda}$ when $K_L \neq 0$;
- $L = \bar{\lambda}, \bar{\lambda} - 2, \dots, 1$ or 0 when $K_L = 0$.

A. A brief look at $K = 1/2$ bands

Let us be specific and discuss ^{19}F and ^{43}Sc . We consider in each case three valence nucleons beyond a closed shell. In ^{19}F the particles are in the $1s-0d$ shell, whereas in ^{43}Sc they are in the $1p-0f$ shell. The energy levels of the lowest bands are given in Table I for the two cases. The results for the two nuclei are striking but different. In ^{19}F , the lowest state is a $I = 1/2^+$ singlet, and at higher energies we get degenerate pairs $(3/2^+, 5/2^+)$, $(7/2^+, 9/2^+)$, $(11/2^+, 13/2^+)$. In ^{43}Sc the ground state is degenerate, and the degenerate pairs are $(1/2^-, 3/2^-)$, $(5/2^-, 7/2^-)$, \dots , $(17/2^-, 19/2^-)$.

If we look at the rotational formula, we find that these results are consistent with a decoupling parameter $a = +1$ for ^{19}F and $a = -1$ for ^{43}Sc . It is easy to show that these are precisely the a -values one obtains with asymptotic Nilsson wave functions. In both cases the odd particle will be in a $\Lambda = 0, \Sigma = 1/2$ state in the asymptotic limit. From the definition of \bar{K} , the state $|\bar{\Lambda} = 0 \Sigma = 1/2\rangle$ can be shown to be equal to $-(-1)^\pi |\Lambda = 0 \Sigma = -1/2\rangle$, where $(-1)^\pi$ is $(+1)$ for an even-parity major shell and (-1) for an odd-parity one. Hence:

$$a = (-1)^\pi \langle \Sigma = +1/2 | J_+ | \Sigma = -1/2 \rangle = (-1)^\pi \quad (13)$$

It has long ago been noted by Bohr and Mottelson [13] that $a = +1$ corresponds to weak coupling of the odd particle to $I = 0^+, 2^+, 4^+, \dots$ states, whereas $a = -1$ corresponds to weak coupling to $I = 1, 3, 5$ states. In the context of the SU(3) model, we would say that the ^{19}F states have an $L(L+1)$ spectrum with only even L 's allowed, and that ^{43}Sc has an $L(L+1)$ spectrum with only odd L 's allowed. It should be emphasized that the purpose of Table I is to compare the results of the $Q \cdot Q$ interaction with the rotational model. To compare with experiment, more realistic interactions including in particular spin-orbit may be required. In this respect, the results in Table I can be considered as the asymptotic limit of large deformation.

At any rate, we have shown that the $Q \cdot Q$ interaction gives the same results for these two $K = 1/2$ bands as does the rotational formula with asymptotic Nilsson wave functions.

Although it is not our intention in this work to fit experiment, rather we wish to work out the consequences of our model, we cannot resist discussing an interesting result for ^{19}F . There is a beautiful example of weak coupling in ^{19}F corresponding to $a = +1$, but it is not the positive parity band discussed above but rather a negative parity band corresponding to a 4-particle 1-hole configuration. This has been discussed by Nazarewicz et al. [25]. In the asymptotic limit the proton hole would be in the Nilsson orbit $[101] \frac{1}{2}$ which would yield $a = 0$. However, the dominance of the $p_{1/2}$ due to spin-orbit interaction causes a to be very close to one. The spectrum looks like the weak coupling of a $p_{1/2}$ hole to the states of the ground state rotational band of ^{20}Ne .

B. Odd-odd nuclei, e.g. ^{22}Na

In Table II we show a fairly detailed list of energy levels for the odd-odd nucleus ^{22}Na obtained with the $Q \cdot Q$ interaction. We show $T = 0$ and $T = 1$ states in separate columns. We use the same parameters as in ^{19}F just to bring out some similarities. If one is interested in a best fit, one should of course have an A dependence in χ .

An striking feature in this table is that many states with diverse $I^\pi T$ assignments are degenerate. This is due to the prevailing $SU(4) \otimes SU(3)$ symmetry. We shall come back to this point at the end of this section but first we compare with the rotational model.

We have underlined $T = 0$ and $T = 1$ rotational bands, and will now discuss them in more detail. Note that the ground state consists of two degenerate states, one with $I = 1^+ T = 0$ and the other with $I = 0^+ T = 1$. Both states have $L = 0$ and the simple spin-independent interaction gives the same energy for $S = 0$ and $S = 1$. Let us first look at the underlined $T = 1$ states. The ground state is $I = 0^+$, the 2^+ state is at 1.588, the 4^+ is at 5.293, etc. If we follow the rotational sequence $I = 0^+, 2^+, 4^+, \dots$ we see a simple rotational behavior:

$$E(I) - E(0_1^+) = AI(I+1); \quad \text{with } A = \frac{\hbar^2}{2I} = \frac{E(2^+) - E(0_1^+)}{6}$$

There is nothing new here.

The excitation energies of the underlined $T = 0$, $I = 1^+, 2^+, 3^+, \dots, 10^+$ states follow the sequence

$$E^*(I) \equiv E(I) - E(1_1^+) = AI(I+1); \quad \text{with } A = \frac{E(2^+) - E(1_1^+)}{6}$$

However the rotational model formula (Eq. (12)) would give a different energy level spacing

$$E^*(I) \equiv E(I) - E(1_1^+) = A'[I(I+1) - 2]; \quad \text{with } A' = \frac{E(2^+) - E(1_1^+)}{4},$$

which is not followed by the above mentioned energy levels in the table. Thus, for the case of $T = 0$ states in odd-odd nuclei we get a clear difference between the rotational formula and $SU(3)$.

We gain further insight by examining the degeneracies associated with the $T = 0$ underlined states in Table II, i.e., those with energy $AI(I+1)$. The even I states up to $I = 8$ are doubly degenerate whereas the $I = 10$ and the odd- I states are singlets. This suggests that there are two bands for which the states with the same I values are degenerate. One band is a $K = 2$ band with all values of I from 2 to 10, and there is nothing anomalous about it. The other band consists of states of angular momentum 1, 2, 4, 6 and 8. For the latter band, the orbital angular momentum of the states are 0, 2, 4, 6 and 8 respectively, and they all have $S = 1$. Their energies can be fit to the formula $E^*(I) = AL(L+1)$ rather than $AI(I+1)$, such that only even L contribute.

Let us now discuss on the basis of $SU(3)$ the degeneracy observed in Table II, limiting the discussion to $T = 0$ and $T = 1$ states (similar arguments would follow for higher isospin states). For ^{22}Na we have 3 protons and 3 neutrons in the $N = 2$ shell. The ground state will correspond to maximal spatial symmetry in coordinate space, i.e., to the $(\lambda, \mu) = (8, 2)$ representation of the $[f] = [4, 2]$ partition. The possible K_L, L values are

- $K_L = 0$: $L = 0, 2, 4, 6, 8$
- $K_L = 2$: $L = 2, 3, 4, 5, \dots, 10$

Since the energy does not depend on K_L (see Eq.(4)), states with equal L -values and different K_L are degenerate. In addition, antisymmetry in spin-isospin space demands that $S = 0$ when $T = 1$, and $S = 1$ when $T = 0$. Therefore, $T = 1$ states with $I = L$, and $T = 0$ states with $I = L, L+1, L-1$ will be degenerate. Thus for the ground state $[4, 2](8, 2)$ representation we find with the same excitation energy $E^*[L] = 3\bar{\chi}L(L+1)$, the following states:

- For $L = 2, 4, 6, 8$
 - two states, each with $T = 0$ and $I = L, L \pm 1$, and
 - two states, each with $T = 1$ and $I = L$,
- For $L = 3, 5, 7, 9, 10$
 - one state with $T = 0$ and $I = L, L \pm 1$, and

– one state with $T = 1$ and $I = L$.

This explains why the state with excitation energy 1.588 MeV (i.e., $L = 2$) appears twice for $T = 0$ and $I = 1, 2, 3$ and twice for $T = 1$ and $I = 2$. The state with excitation energy 3.176 MeV (i.e., $L = 3$) appears once with $T = 0, I = 2, 3, 4$ and once with $T = 1, I = 3$. The next state of this representation is at 5.293 MeV (i.e., $L = 4$), and according to the above discussion should appear twice for $T = 0$ and $I = 3, 4, 5$ and twice for $T = 1$ and $I = 4$.

Surprisingly though there are more degeneracies at 5.293 MeV, namely one $T = 0$ state with $I = 3$ and three $T = 1$ states with $I = 2, 3, 4$. This is due to an additional degeneracy of $[4, 2] (8, 2) L = 4$ with the $[4, 1, 1] (9, 0) L = 3$ state that corresponds to total symmetry in spin-isospin space (i.e., $T = 0, S = 0$ or $T = 1, S = 1$). The allowed K_L, L values in this representation are $K_L = 0, L = 1, 3, 5, 7, 9$, and the excitation energy for a given L -value, $E^* [(90)L] - E_{GS}^* [0] = \bar{\chi} [24 + 3L(L + 1)]$, is shared by states with $T = 0, I = L$ and with $T = 1, I = L, L \pm 1$. Thus the states that belong to this representation for $L = 1$ are the states at 2.647 MeV with $T = 0, I = 1$ and $T = 1, I = 0, 1, 2$, while for $L = 3$ we get the states at 5.294 MeV previously discussed with $T = 0, I = 3$ and with $T = 1, I = 4$, plus the states $T = 1, I = 2, 3$. The next states with $L = 5$ ($E^* = 10.055$) appear for $T = 0, I = 5$, $T = 1, I = 4, 5, 6$, and are degenerate with lower angular momentum states corresponding to $K_L = 1, L = 2$ in the $(6, 3)$ representation (The $L = 1$ states in this last representation have 9 MeV excitation energy). By the same token one can explain the remaining energy levels in the table. To the best of our knowledge there has been no discussion previously of these additional degeneracies corresponding to different values in different representations.

Experimentally the lowest band in ^{22}Na has $K = 3$. In the Nilsson scheme when we fill the lowest $N = 2, K = 1/2$ level we reach ^{20}Ne . To form ^{22}Na we put the odd neutron and odd proton into the $K = 3/2$ level and the Gallagher Moszkowski rule favors $K = 3$ over $K = 0$ for the lowest band [26]. However, with pure $Q \cdot Q$ as seen in Table II, the lowest $I = 3^+$ state comes out at 1.588 MeV of excitation. Clearly, the limitations of the SU(3) formula for energy levels are more apparent when one examines the spectra of odd-even and odd-odd nuclei rather than limiting oneself to even-even nuclei. The main deficiency is the absence of a spin-orbit interaction in the SU(3) model. For even-even nuclei the lowest lying levels are dominantly $S = 0$ states but this is not the case for $T = 0$ states of odd-odd nuclei.

IV. CONVERGENCE WITH A $Q \cdot Q$ INTERACTION

We now come to the last topic of this work – how to achieve convergence with a $Q \cdot Q$ interaction. When we remove the momentum dependent terms from $Q \cdot Q$ and go back to the \mathbf{r} space $Q^r \cdot Q^r$, we can mix major shells. Therefore, this coordinate space interaction combines the advantages of the algebraic Elliott's model, with the possibility of studying intruder states and admixtures of higher shells in the ground state.

There is a general belief that if we go to larger and larger spaces the results will diverge. This is because the $Q^r \cdot Q^r$ interaction increases its strength as the distance between two nucleons increases. However, we wish to show in this work that we can get around this problem. Just as people do all the time in G-matrix calculations, we can modify the interaction as we change the model space. If we allow up to $n\hbar\omega$ excitations in the model space we can make the strength of the $Q^r \cdot Q^r$ depend on n

$$V = -\frac{\chi_n}{2} Q^r \cdot Q^r .$$

A simple scheme for getting convergence is to demand that the energy of the $I = 2_1^+$ state in an open shell nucleus comes out correctly (i.e., agrees with experiment) for each n . We have applied this scheme to the $I = 0^+, 1^+$ and 2^+ (all $T = 0$) states in ^8Be . These are shown in Tables III, IV, and V, respectively. In each table the results are given in a $0\hbar\omega$ space ($n = 0$), $(0 + 2)\hbar\omega$ space ($n = 2$), and $(0 + 2 + 4)\hbar\omega$ space ($n = 4$). In order to get the $I = 2_1^+$ state to come out correctly we had to steadily decrease χ with increasing n . The values for $n = 0, 2$, and 4 are respectively 0.5216, 0.4119, and 0.3369 MeV fm $^{-4}$.

The calculations have been performed using the OXBASH program [27]. In this program the effects of spurious states are removed using the Gloeckner-Lawson method [28]. In this method the spurious states are pushed up to a very high energy. This is done by diagonalizing the modified Hamiltonian for a system of A nucleons

$$H' = H_{SM} + \lambda_{CM} \left[\frac{\mathbf{P}^2}{2Am} + \frac{1}{2} m A \omega^2 \mathbf{R}^2 - \frac{3}{2} \hbar \omega \right] \quad (14)$$

where H_{SM} is the usual shell model Hamiltonian and \mathbf{P} and \mathbf{R} are the position vectors for the center of mass. By making λ_{CM} very large, the spurious states corresponding to center of mass motion will be pushed up to a very high energy. They will be well separated from the lower lying physical states.

Let us first discuss the calculations up to $2\hbar\omega$, the results of which are given in the tables III, IV and V. These excitations are of two types, we can either excite one particle through 2 major shells ($1p-1h$) or we can excite two nucleons through one major shell ($2p-2h$). The ($1p-1h$) excitations can be regarded as giant resonance states built upon the valence states as have indeed been studied in the context of symplectic symmetry [2]. The giant resonance states are generally at high excitation energies but their admixtures into the valence states can lead to important effects. For example, the isoscalar $E2$ effective charge needed to fit experiments in valence space calculations is about a factor two larger than the bare charge and this can be understood in terms of small admixtures of the $2\hbar\omega$ ($1p-1h$) states into the basis valence states.

We next consider the $2p-2h$ states. In some nuclei some states of this type come much lower in energy than the $2\hbar\omega$ estimate. They may intertwine with low lying valence states. In such cases these $2p-2h$ states or more generally, $np-nh$ states, are called *intruder states*. In previous calculations [29] we have shown that there are such low lying intruders in ^{10}Be , ^{12}C and ^{16}O , but actually not in ^8Be .

The reason that in some nuclei the intruders come low in energy and in others they do not, can be understood in the context of the Nilsson model. The optimum way to have a low lying intruder is to lift two nucleons from a Nilsson orbit whose energy increases with deformation (upgoing level) and to put them into a Nilsson orbit whose energy decreases with deformation (downgoing level). For ^{10}Be , ^{12}C and ^{16}O we can remove nucleons from upgoing levels in the $0p$ -shell, but in the case of ^8Be the valence levels are depleted and we would have to remove nucleons from a downgoing level.

Before discussing the energy levels we will make some comments about the occupancies. It had been previously noted by Fayache et al. [30] that if one allows only $2\hbar\omega$ admixtures with the $Q \cdot Q$ interaction then the shell model matrix reduces into two parts. First, we have states which are admixtures of valence states (no particles excited to higher shells) and states in which one nucleon is excited through two major shells, and second we have states in which two particles are excited through one major shell. There is no mixing in between the ($0p-0h+1p-1h$) states and the $2p-2h$ states. This is because of the 'parity' selection rule that $Q \cdot Q$ cannot excite two nucleons from an even (odd) parity major shell to an odd (even) major shell.

If we look at Tables III, IV, and V under the columns $(0+2)\hbar\omega$ we see several states which have 100% $2\hbar\omega$ configurations. These are precisely the $2p-2h$ states which are uncoupled from the rest. When we allow $4\hbar\omega$ admixtures the $2p-2h$ states admix with states in which one nucleon is excited through one major shell and the other through three major shells. We therefore no longer get 100% $2\hbar\omega$ for these states, but they are still uncoupled from states which have mainly valence configurations.

In more detail, for $I = 0^+$ in Table III, in the $(0+2)\hbar\omega$ column the ground state has 21.77% $2\hbar\omega$ admixtures. The next four states have smaller $2\hbar\omega$ admixtures, but the state at 30.951 MeV has an 88.89% admixture. This is clearly a state which is dominantly a $1p-1h$ state in which a nucleon has been excited through 2 major shells. This state can be easily distinguished from the $2p-2h$ states at 32.214 MeV and 34.409 MeV. The latter have 100% $2\hbar\omega$ configurations. As mentioned before there is no mixing, at the $2\hbar\omega$ level between the ($0p-0h+1p-1h$) states and the $2p-2h$ states via a $Q \cdot Q$ interaction.

States with 100% occupancy are also seen in Tables IV and V corresponding to $I = 1^+$ and 2^+ . These all lie in the energy range 30-35 MeV, and are clearly $2p-2h$ states. As mentioned before there are no low lying intruders in ^8Be . These $2p-2h$ states are close in energy with the (dominantly) $1p-1h$ states for ^8Be .

When we go to the $(0+2+4)\hbar\omega$ column the results are not so striking – we do not see 100% of any configuration. But we can still distinguish the ($0p-0h+1p-1h$) states from the ($2p-2h+2p-2h \otimes 1p-1h$) states. For the latter the sum of the $2\hbar\omega + 4\hbar\omega$ occupancy should be 100%. For the $I = 0^+$ states in Table III this is not the case for the state at 26.225 MeV (71.5%) but it is the case for states at 32.085 MeV and 34.200 MeV. Similar states can be found for $I = 1^+$ and 2^+ , i.e. states where the $2\hbar\omega + 4\hbar\omega$ occupancy is 100%. This confirms that with $Q \cdot Q$ one gets a separation of different classes of states.

We now discuss the energy levels as a function of n , the number of $\hbar\omega$ excitations. While there are rather large deviations in going from $n = 0$ to $n = 2$, there is excellent convergence for many states in comparing $n = 2$ and $n = 4$. The percentage deviation for the $I = 0^+$ case for the first 4 states (up to about 20 MeV) are respectively 0.77, 2.22, 2.75, and 3.93%. For the next state, which is at 26.225 MeV in the $(0+2+4)\hbar\omega$ calculation, the percentage deviation is large 18.02%. But if we examine this state we see that it is mainly a $2\hbar\omega$ excitation state, not present in the $0\hbar\omega$ calculation. It corresponds to a $1p-1h$ excitation through 2 major shells, as opposed to many other $2\hbar\omega$ states which correspond to two nucleons being excited through one major shell.

We see that the convergence between $(0+2)\hbar\omega$ and $(0+2+4)\hbar\omega$ holds to surprisingly high energies. For example for $I = 1^+$ at the $(0+2)\hbar\omega$ energy level there are five consecutive $2p-2h$ states between 30.722 MeV and 34.503 MeV. The % deviations in the energies relative to the $(0+2+4)\hbar\omega$ calculations are respectively 10.13, 9.19, 4.84, 2.01 and 1.87%.

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Table I. Energy levels (MeV) of excited states corresponding to the $K = 1/2$ ground state bands in ^{19}F and ^{43}Sc with the $-\chi Q \cdot Q$ interaction.

$^{19}\text{F}^a$		$^{43}\text{Sc}^b$	
I^π	E^*	I^π	E^*
$(1/2)^+$	0	$(1/2)^-$	0
$(3/2)^+$	1.588	$(3/2)^-$	0
$(5/2)^+$	1.588	$(5/2)^-$	0.679
$(7/2)^+$	5.295	$(7/2)^-$	0.679
$(9/2)^+$	5.295	$(9/2)^-$	1.900
$(11/2)^+$	11.118	$(11/2)^-$	1.900
$(13/2)^+$	11.118	$(13/2)^-$	3.664
		$(15/2)^-$	3.664
		$(17/2)^-$	5.971
		$(19/2)^-$	5.971

^a For ^{19}F we use $\chi = 0.1841$ ($\bar{\chi} = 0.0882$)

^b For ^{43}Sc we use $\chi = 0.0294$ ($\bar{\chi} = 0.0218$)

Table II. $T = 0$ and $T = 1$ energy levels (MeV) of ^{22}Na calculated with the $-\chi Q \cdot Q$ interaction ^a. Only the first six levels for each I^π are shown.

I^π	$T = 0$ states	$T = 1$ states	I^π	$T = 0$ states	$T = 1$ states
0^+	8.999	<u>0.000</u>	6^+	7.941	10.059
	12.176	2.647		<u>11.117</u>	<u>11.117</u>
	12.176	8.999		11.117	11.118
	13.235	9.000		14.824	16.412
	16.410	12.176		16.411	16.412
	16.411	12.176		16.411	16.412
1^+	<u>0.000</u>	2.647	7^+	11.117	14.823
	1.588	8.999		11.117	16.940
	1.588	8.999		<u>14.823</u>	19.587
	2.647	10.059		16.941	19.587
	9.000	10.059		19.058	19.587
	9.000	10.059		19.059	19.587
2^+	<u>1.588</u>	<u>1.588</u>	8^+	14.823	16.941
	1.588	1.588		<u>19.058</u>	<u>19.058</u>
	3.176	2.647		19.059	19.059
	8.999	5.294		22.763	22.767
	10.059	9.000		23.292	23.293
	10.059	9.000		23.293	23.293
3^+	1.588	3.176	9^+	19.058	23.822
	1.588	5.293		19.058	25.939
	<u>3.177</u>	10.058		<u>23.822</u>	26.470
	5.294	10.058		25.940	27.527
	5.294	11.646		26.469	27.527
	5.294	11.646		27.528	29.644
4^+	3.176	<u>5.293</u>	10^+	23.823	25.942
	<u>5.293</u>	5.293		<u>29.117</u>	<u>29.117</u>
	5.293	5.293		30.705	30.706
	7.941	10.059		32.293	32.294
	11.647	11.647		33.881	32.294
	11.647	11.647			33.882
5^+	5.294	7.941			
	5.294	10.059			
	<u>7.941</u>	13.763			
	10.059	13.763			
	11.118	13.763			
	11.118	13.763			

^a In this table and in the following tables, the same value of χ (and of $\bar{\chi}$) was used for ^{22}Na as for ^{19}F .

Table III. The energies E^* (MeV) and percentages of $2\hbar\omega$ and $4\hbar\omega$ occupancies of the $J = 0^+$ $T = 0$ states in ^8Be in three different model spaces. The last column gives the % energy deviation between the $(0 + 2)$ $\hbar\omega$ and $(0 + 2 + 4)$ $\hbar\omega$ calculations.

$0 \hbar\omega$	$(0 + 2) \hbar\omega$		$(0 + 2 + 4) \hbar\omega$			% deviation
$\chi = 0.5216$	$\chi = 0.4119$		$\chi = 0.3369$			
E^*	E^*	% $2\hbar\omega$	E^*	% $2\hbar\omega$	% $4\hbar\omega$	
0.00	0.000	21.77	0.000	24.60	10.74	
9.12	11.458	10.28	11.370	10.90	5.69	0.77
12.16	16.231	1.91	15.879	2.07	3.55	2.22
15.20	18.352	2.96	17.860	2.53	3.16	2.75
17.23	20.147	2.62	19.385	2.10	2.98	3.93
	30.951	88.89	26.225	50.93	20.56	18.02
	32.214	100.00	29.701	77.30	19.41	8.46
	32.396	92.36	32.085	86.13	13.87	0.97
	34.409	100.00	34.200	86.82	13.18	0.61
	38.702	91.66	35.928	70.75	15.45	7.72

Table IV. Same as Table III but for the $J = 1^+$ states.

$0 \hbar\omega$	$(0 + 2) \hbar\omega$		$(0 + 2 + 4) \hbar\omega$			% deviation
$\chi = 0.5216$	$\chi = 0.4119$		$\chi = 0.3369$			
E^*	E^*	% $2\hbar\omega$	E^*	% $2\hbar\omega$	% $4\hbar\omega$	
9.12	11.458	10.28	11.371	10.90	5.69	0.77
11.15	13.734	8.85	13.587	8.92	4.87	1.08
15.20	18.353	2.96	17.861	2.53	3.16	2.75
17.23	20.148	2.62	19.385	2.10	2.98	3.94
	30.722	100.00	27.896	78.69	21.31	10.13
	32.992	100.00	30.215	79.30	20.70	9.19
	33.294	100.00	31.756	82.55	17.45	4.84
	34.409	100.00	33.731	86.28	13.72	2.01
	34.503	100.00	33.869	83.31	16.59	1.87
	35.357	99.84	34.200	86.81	13.19	3.38
	37.666	92.98	35.707	74.99	14.33	5.49
	38.702	91.65	35.927	70.75	15.44	7.72
	40.174	100.00	38.724	85.12	14.80	3.74
	40.485	99.97	39.313	86.37	13.63	2.98
	40.706	100.00	39.331	86.38	13.63	3.50

Table V. Same as Table III but for the $J = 2^+$ states.

$0 \hbar\omega$	$(0 + 2) \hbar\omega$		$(0 + 2 + 4) \hbar\omega$			% deviation
$\chi = 0.5216$	$\chi = 0.4119$		$\chi = 0.3369$			
E^*	E^*	$\%2\hbar\omega$	E^*	$\%2\hbar\omega$	$\%4\hbar\omega$	
3.04	3.042	21.42	3.038	23.81	9.94	0.13
9.12	11.458	10.28	11.370	10.90	5.69	0.77
11.15	13.734	8.85	13.586	8.92	4.87	1.09
12.15	16.197	8.99	15.880	2.07	3.55	2.00
14.18	16.231	1.91	15.949	8.31	4.21	1.77
15.20	18.353	2.96	17.859	2.53	3.16	2.77
17.23	20.148	2.62	19.385	2.10	2.98	3.94
	31.711	82.81	27.146	51.37	20.15	16.82
	32.214	100.00	30.215	79.30	20.70	6.62
	32.992	100.00	31.714	80.12	18.91	4.03
	33.962	99.68	32.085	86.13	13.87	5.85
	34.410	100.00	33.869	83.31	16.60	1.60
	35.357	99.84	34.201	86.81	13.19	3.38
	37.668	92.98	35.707	75.00	14.33	5.49